

Abstract Submitted  
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**Intrinsic ferromagnetism at AlN-MgB<sub>2</sub> interfaces** YOSHIHIRO GOHDA, SHINJI TSUNEYUKI, Univ. of Tokyo — Spin polarization without magnetic elements is possible utilizing dangling bonds. In particular, nitrogen-dangling bonds of cation vacancies are responsible for spin polarization in nitride semiconductors. Enhancement of ferromagnetism due to cation vacancies by Gd dopants has also been found [1], which is consistent with colossal magnetic moments per Gd observed in experiments. However, randomness of point-defect distribution is not feasible to control magnetisation. In this situation, ordered structures of spin sites are highly desirable for the control of magnetization. In this study, we demonstrate by means of first-principles calculations that nitride-boride interfaces could be a candidate for such ordered spin sites. Partially occupied N  $p$  states at AlN-MgB<sub>2</sub>(0001) interfaces exhibits two-dimensional spin polarization, which cannot be anticipated from the atomic structure because the N dangling bonds are apparently saturated by Mg. Hund's coupling of the two N  $p_{||}$  orbitals as well as high density of spin-unpolarized states at the Fermi energy contribute to strong itinerant ferromagnetism. Roles of metal-induced gap states [2] will also be discussed.

[1] Y. Gohda and A. Oshiyama, Phys. Rev. B 78, 161201(R) (2008).

[2] Y. Gohda, S. Watanabe, and A. Groß, Phys. Rev. Lett. 101, 166801 (2008).

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